LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110923\
Data File : BM042681.D
Acq On : 09 Nov 2023 20:57
Operator : MA/JU
Sample : 05270-01 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
OR-3-110623

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042681.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.375	400	406	415	rBV	131390	210947	18.35%	2.125%
2	7.010	678	684	696	rBV	113304	217341	18.90%	2.189%
3	7.845	820	826	839	rBV	164979	280860	24.43%	2.829%
4	9.045	1024	1030	1046	rBV	62613	131711	11.46%	1.327%
5	9.933	1175	1181	1199	rBV3	22240	79058	6.88%	0.796%
6	10.657	1295	1304	1323	rBV	192069	354349	30.82%	3.569%
7	13.121	1717	1723	1733	rBV	171620	268942	23.39%	2.709%
8	14.227	1906	1911	1917	rBV	27406	44699	3.89%	0.450%
9	14.498	1950	1957	1965	rBV	284880	425094	36.97%	4.282%
10	14.563	1965	1968	1972	rVB	11089	16199	1.41%	0.163%
11	14.904	2017	2026	2031	rBV3	8820	18334	1.59%	0.185%
12	15.551	2129	2136	2146	rBV2	18895	33566	2.92%	0.338%
13	15.998	2203	2212	2224	rBV	138376	226606	19.71%	2.282%
14	16.545	2298	2305	2310	rBV3	6525	11620	1.01%	0.117%
15	17.074	2392	2395	2404	rVB	8205	12007	1.04%	0.121%
16	17.251	2419	2425	2429	rBV	352087	501670	43.63%	5.053%
17	17.292	2429	2432	2442	rVV	168802	252397	21.95%	2.542%
18	17.386	2443	2448	2459	rVV	43262	78621	6.84%	0.792%
19	17.680	2491	2498	2508	rVB4	12662	27852	2.42%	0.281%
20	18.109	2565	2571	2578	rBV3	60245	143770	12.50%	1.448%
21	18.174	2578	2582	2589	rVV	44460	72402	6.30%	0.729%
22	18.256	2591	2596	2600	rVV	17897	28067	2.44%	0.283%
23	18.321	2600	2607	2611	rVV2	65183	124440	10.82%	1.253%
24	18.356	2611	2613	2619	rVB	26937	35212	3.06%	0.355%
25	18.627	2653	2659	2664	rBV2	19369	33605	2.92%	0.338%
26	18.915	2704	2708	2711	rVB2	11769	15489	1.35%	0.156%
27	18.956	2712	2715	2720	rVB3	12191	15620	1.36%	0.157%
28	19.033	2722	2728	2733	rBV	37965	66409	5.78%	0.669%
29	19.168	2748	2751	2753	rBV3	13841	17696	1.54%	0.178%
30	19.309	2769	2775	2781	rBV	508232	680658	59.20%	6.856%
31	19.386	2785	2788	2797	rVV4	39490	80530	7.00%	0.811%
32	19.462	2797	2801	2808	rVB	32802	51157	4.45%	0.515%
33	19.556	2815	2817	2826	rVB4	19050	43063	3.75%	0.434%
34	19.633	2826	2830	2833	rBV2	61368	94715	8.24%	0.954%
35	19.674	2833	2837	2844	rVV	472022	633699	55.12%	6.383%
36	19.739	2844	2848	2853	rVB2	26226	45463	3.95%	0.458%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110923\
Data File : BM042681.D
Acq On : 09 Nov 2023 20:57
Operator : MA/JU
Sample : 05270-01 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
OR-3-110623

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.868	2864	2870	2878	rBV	392081	519932	45.22%	5.237%
38	19.992	2886	2891	2898	rVB3	38675	92131	8.01%	0.928%
39	20.133	2909	2915	2917	rBV4	33170	66630	5.80%	0.671%
40	20.168	2917	2921	2926	rVB	82154	119355	10.38%	1.202%
41	20.268	2934	2938	2941	rBV	69215	87735	7.63%	0.884%
42	20.321	2941	2947	2952	rVV3	38842	75754	6.59%	0.763%
43	20.462	2968	2971	2975	rBV	34586	44779	3.89%	0.451%
44	20.509	2976	2979	2986	rVB2	37069	54083	4.70%	0.545%
45	21.080	3073	3076	3079	rBV	48371	69549	6.05%	0.700%
46	21.156	3086	3089	3097	rBV3	33420	64908	5.65%	0.654%
47	21.433	3129	3136	3140	rBV2	612937	1149728	100.00%	11.580%
48	21.474	3140	3143	3148	rVB	256594	335007	29.14%	3.374%
49	23.080	3410	3416	3422	rBV	201134	547919	47.66%	5.519%
50	23.597	3499	3504	3514	rVB	144015	288288	25.07%	2.904%
51	23.703	3517	3522	3531	rVB	183147	350753	30.51%	3.533%
52	23.809	3534	3540	3546	rBV	349545	688173	59.86%	6.931%

Sum of corrected areas: 9928592

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110923\
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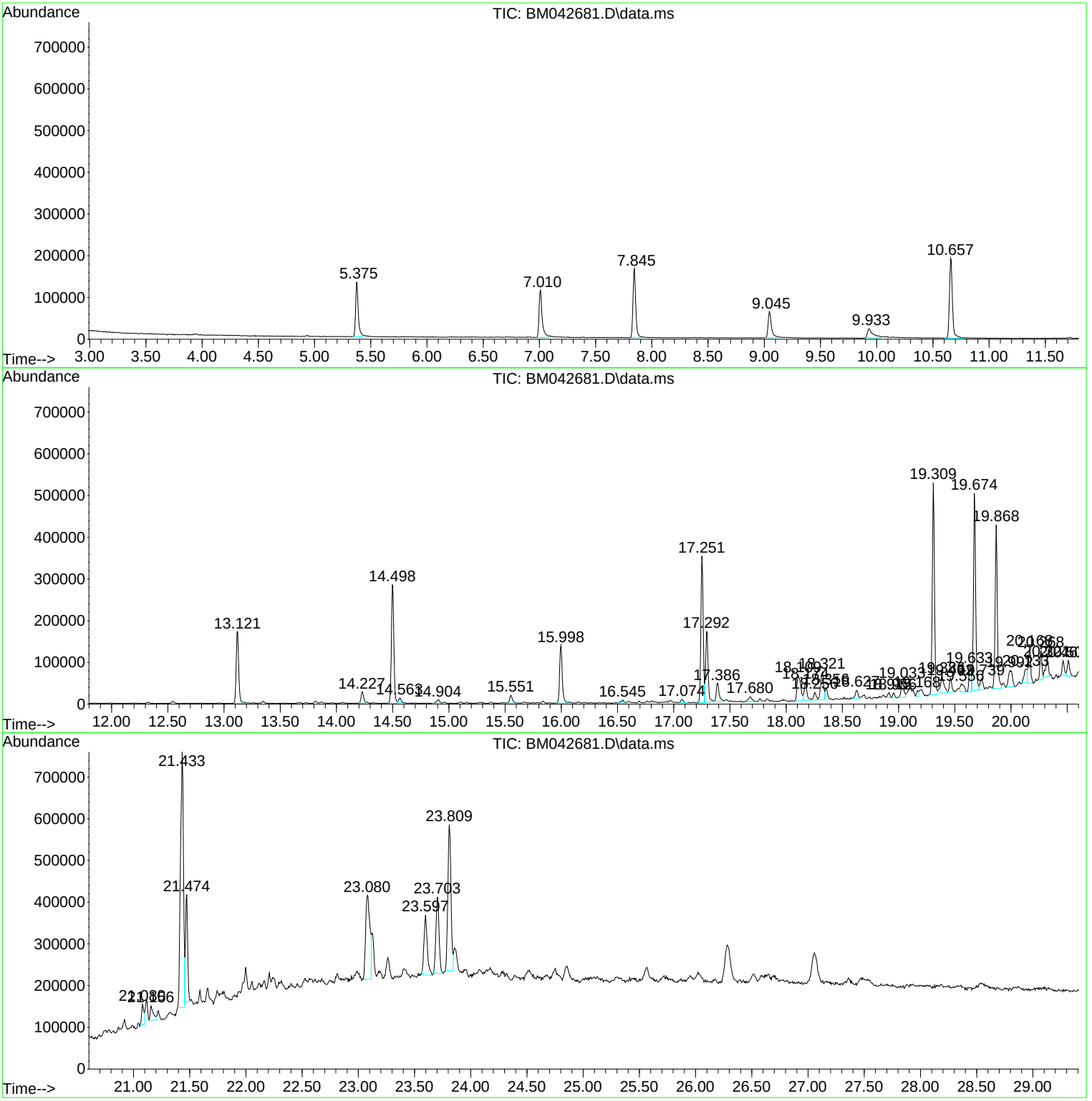
Sample : 05270-01 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
OR-3-110623

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110923\
Data File : BM042681.D
Acq On : 09 Nov 2023 20:57
Operator : MA/JU
Sample : 05270-01 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
OR-3-110623

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

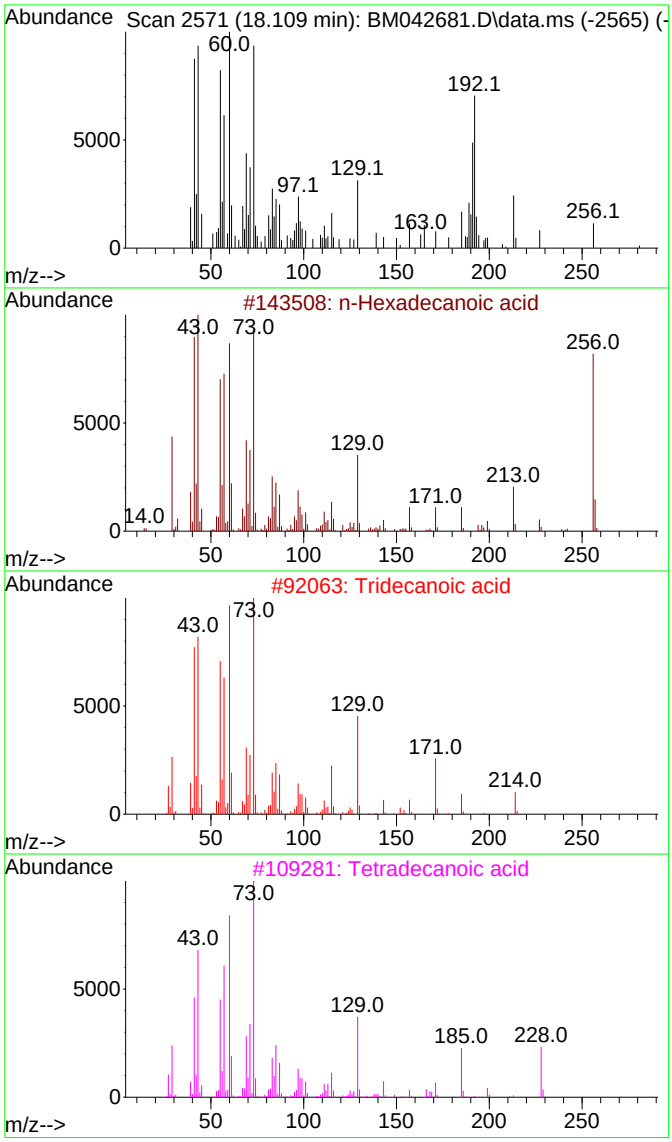
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

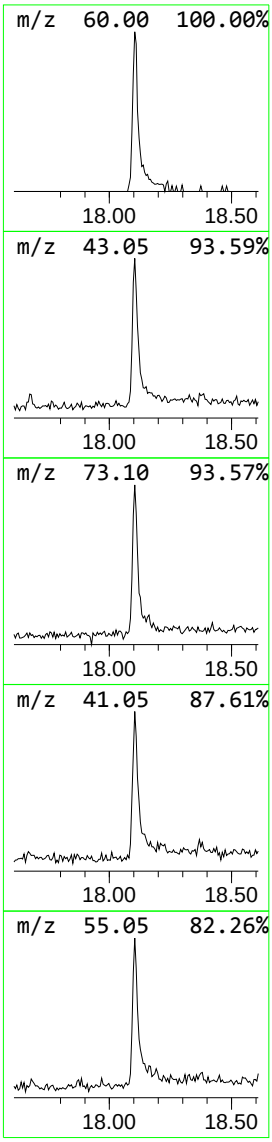
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.109	5.73 ng	143770	Phenanthrene-d10	17.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	70
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	46
4	Undecanoic acid	186	C11H22O2	000112-37-8	46
5	n-Decanoic acid	172	C10H20O2	000334-48-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110923\
Data File : BM042681.D
Acq On : 09 Nov 2023 20:57
Operator : MA/JU
Sample : 05270-01 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
OR-3-110623

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

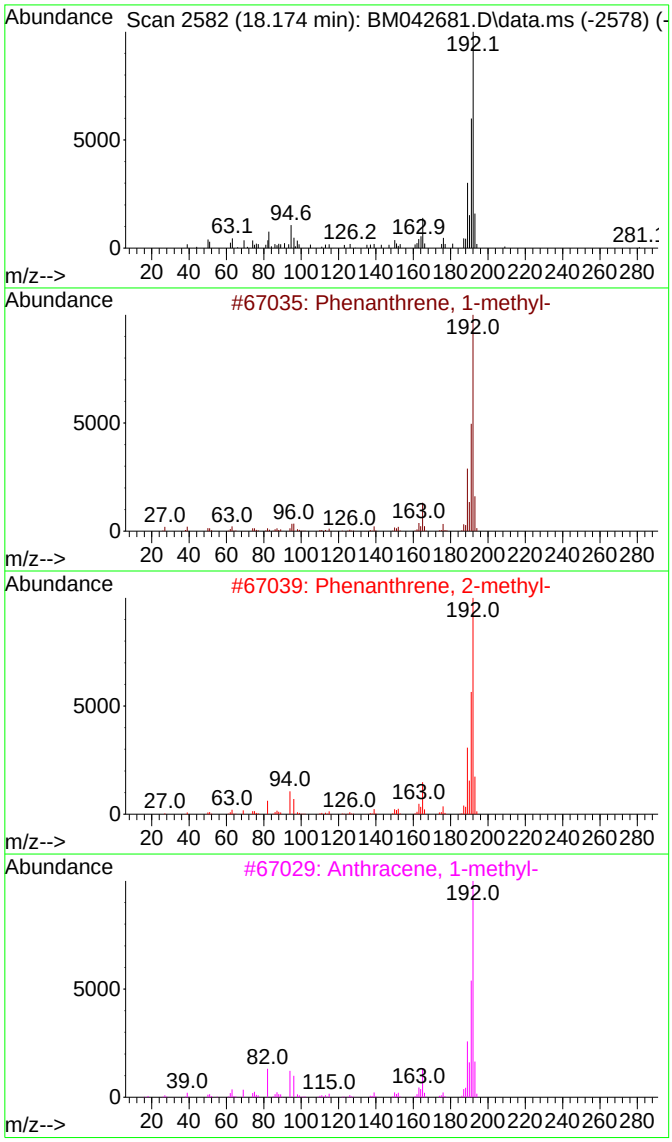
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

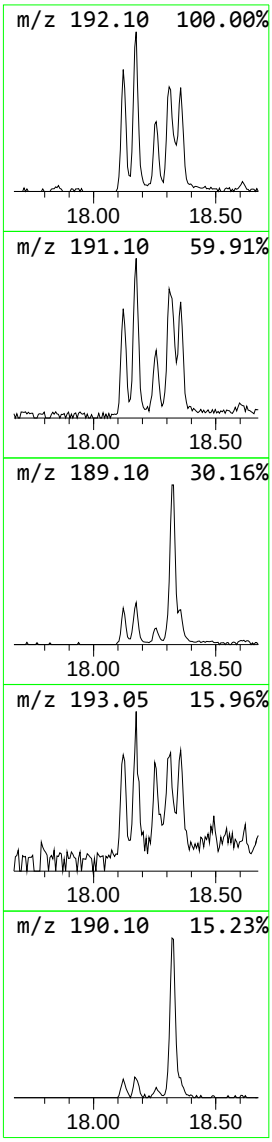
****

Peak Number 2 Phenanthrene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.174	2.89 ng	72402	Phenanthrene-d10	17.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	93
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110923\
Data File : BM042681.D
Acq On : 09 Nov 2023 20:57
Operator : MA/JU
Sample : 05270-01 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
OR-3-110623

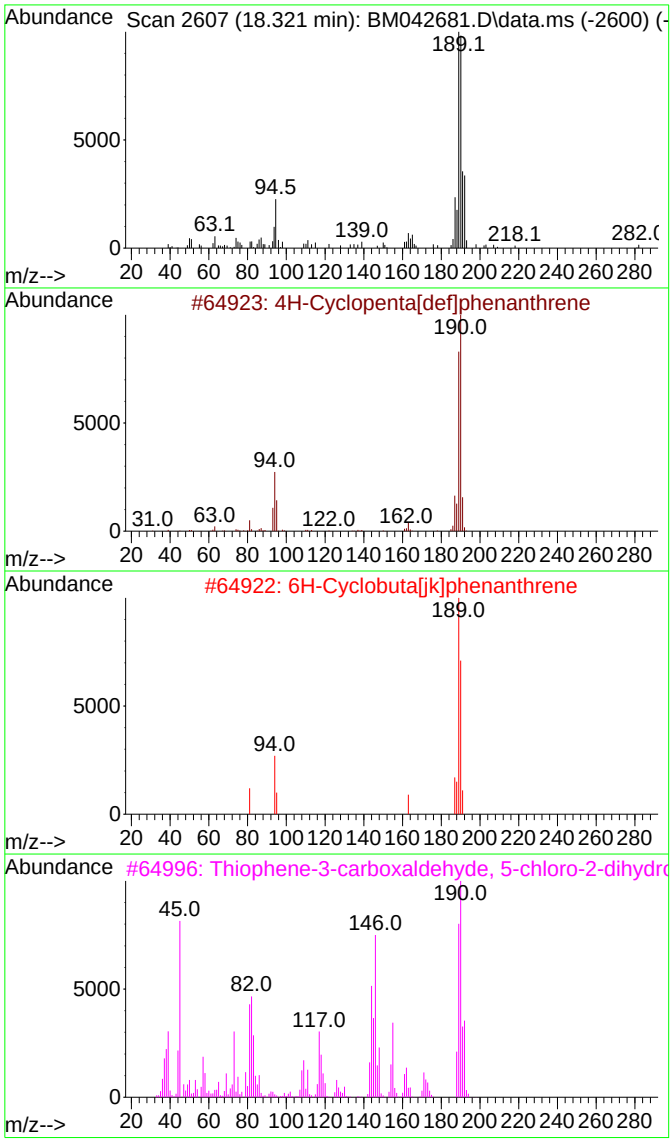
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

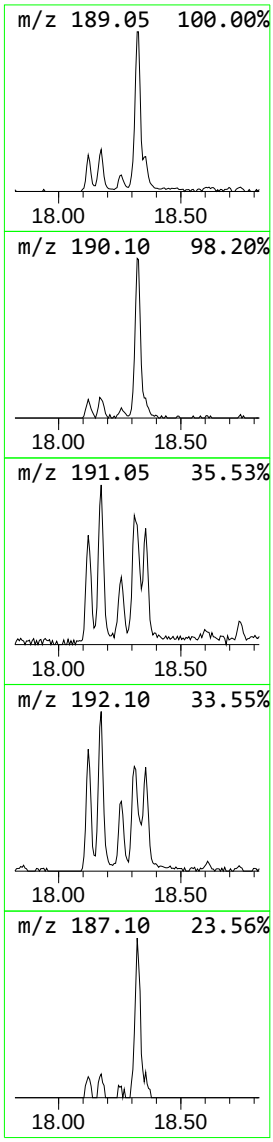
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.321	4.96 ng	124440	Phenanthrene-d10	17.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	83
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	72
3	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	64
4	Methyl diselenide	190	C2H6Se2	007101-31-7	49
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110923\
Data File : BM042681.D
Acq On : 09 Nov 2023 20:57
Operator : MA/JU
Sample : 05270-01 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
OR-3-110623

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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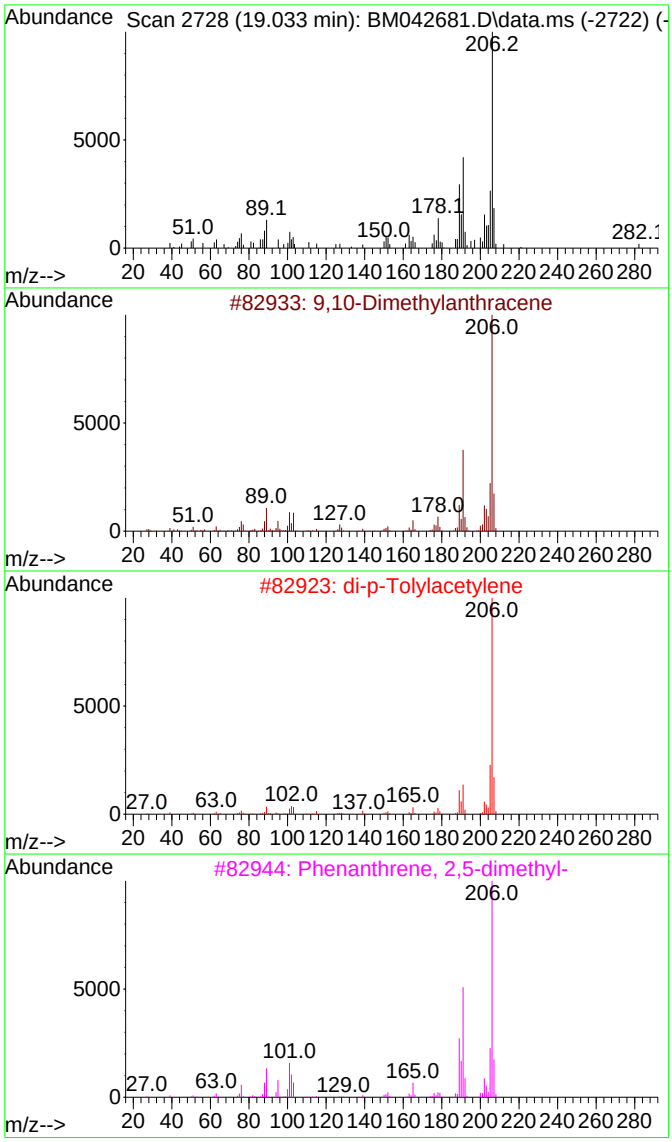
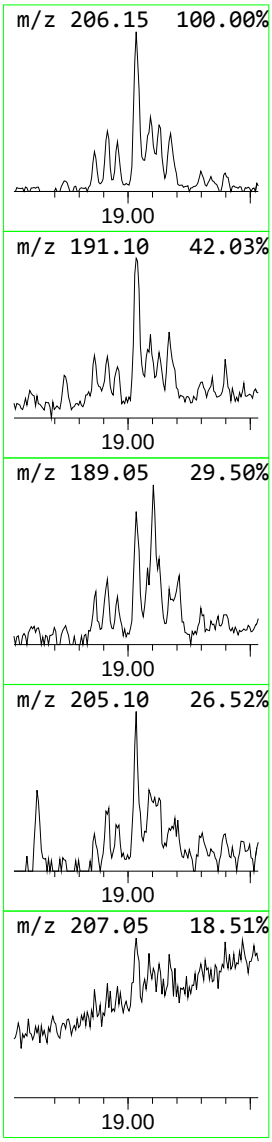
Peak Number 4 9,10-Dimethylanthracene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.033	2.65 ng	66409	Phenanthrene-d10	17.251

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Dimethylanthracene	206	C16H14	000781-43-1	96
2	di-p-Tolylacetylene	206	C16H14	002789-88-0	94
3	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	91
4	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	90
5	3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110923\
Data File : BM042681.D
Acq On : 09 Nov 2023 20:57
Operator : MA/JU
Sample : 05270-01 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
OR-3-110623

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

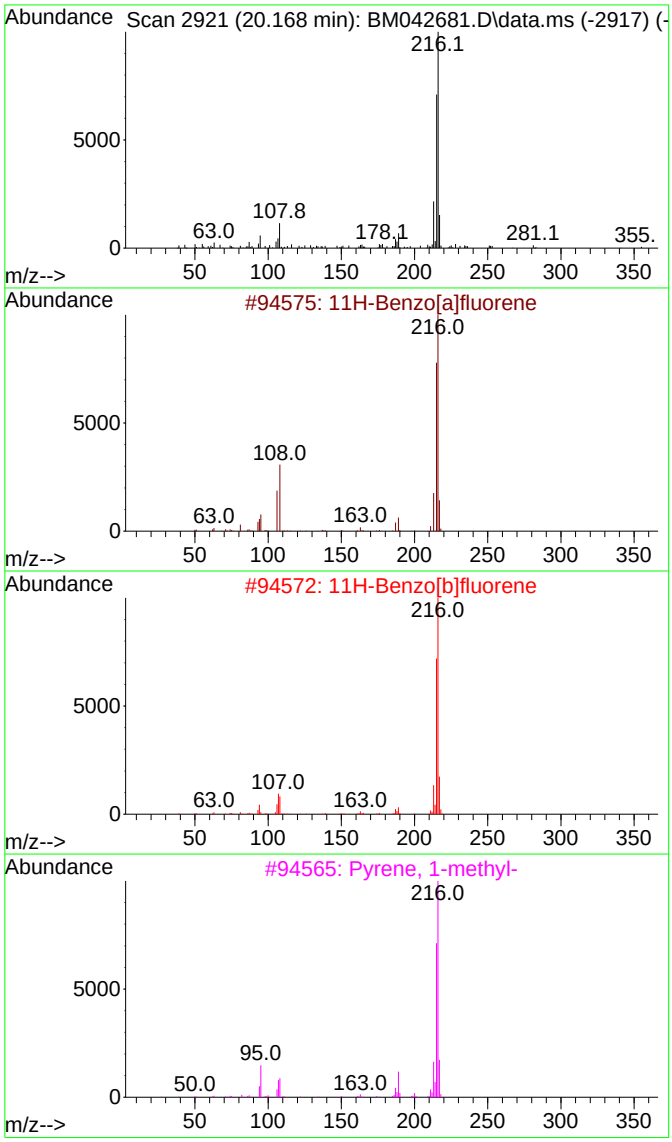
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

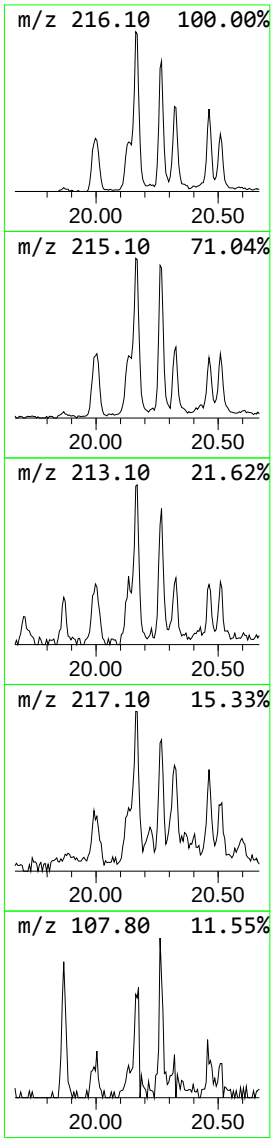
****

Peak Number 5 11H-Benzo[a]fluorene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.168	2.08 ng	119355	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	83
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	83
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	74
5	6H-Thiazolo[5,4-e]indole, 2,7,8-...	216	C12H12N2S	1000338-32-0	72





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Data File : BM042681.D
Acq On : 09 Nov 2023 20:57
Operator : MA/JU
Sample : 05270-01 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
OR-3-110623

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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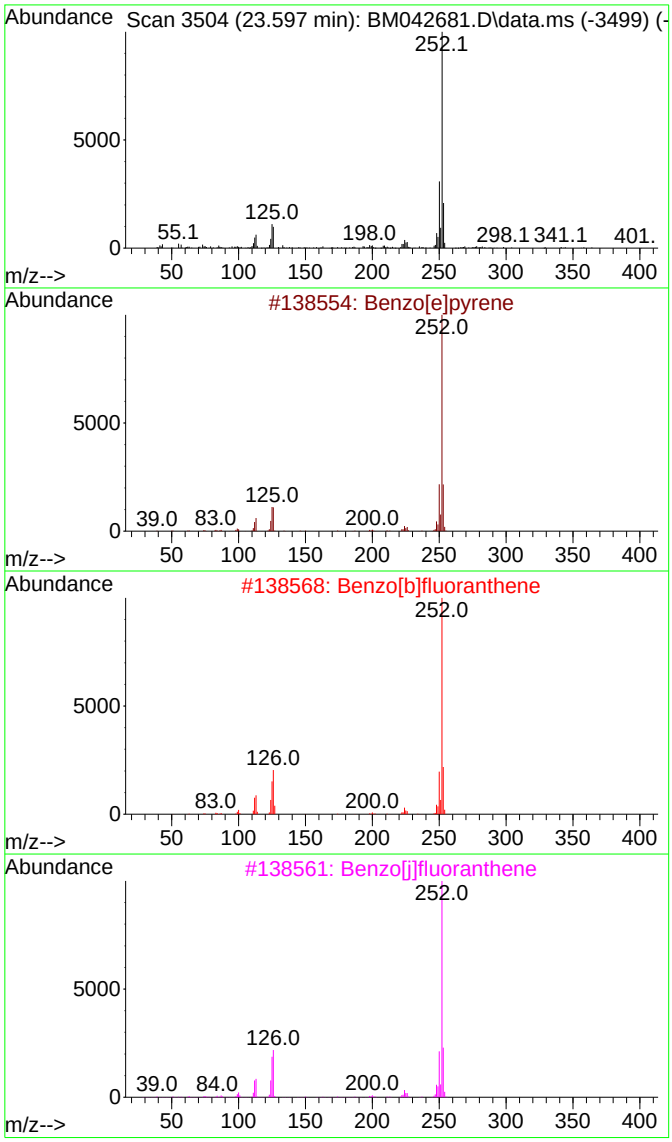
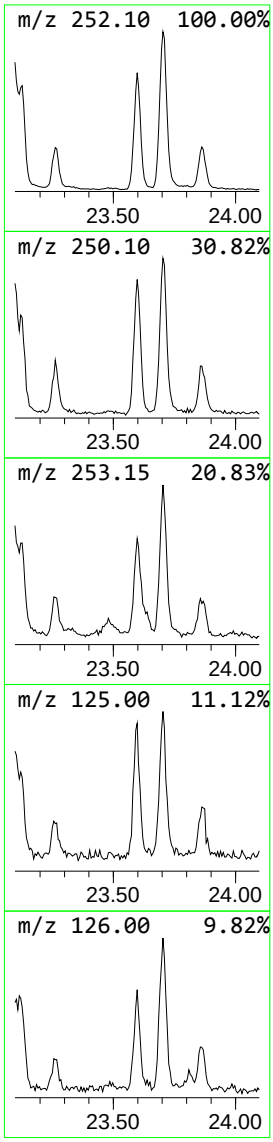
Peak Number 6 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.597	8.38 ng	288288	Perylene-d12	23.809

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	93
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM110923\
Data File : BM042681.D
Acq On : 09 Nov 2023 20:57
Operator : MA/JU
Sample : 05270-01 5X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
OR-3-110623

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Hexadecanoic ...	18.109	5.7	ng	143770	4	17.251	501670	20.0
Phenanthrene, 1...	18.174	2.9	ng	72402	4	17.251	501670	20.0
4H-Cyclopenta[d...	18.321	5.0	ng	124440	4	17.251	501670	20.0
9,10-Dimethylan...	19.033	2.6	ng	66409	4	17.251	501670	20.0
11H-Benzo[a]flu...	20.168	2.1	ng	119355	5	21.433	1149730	20.0
Benzo[e]pyrene	23.597	8.4	ng	288288	6	23.809	688173	20.0